Chlorfenac 85-34-7 | DTXSID2040284

Model	Perform	anca
IVIOCEI	renonn	ance

Model	Data

Weighted KNN model

5-fold CV	5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.84	0.55	0.85	0.53	0.83	0.64	

Model Results

Predicted value: 3.49

Global applicability domain: Inside

Local applicability domain index: 4.22e-01

Confidence level: 7.12e-01

Nearest Neighbors from the Training Set

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Dalapon-sodium Measured: 7.24 Predicted: 5.61

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Trichloroacetic acid Measured: 1.70 Predicted: 2.22

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3,4-Dichlorobenzoic acid Measured: 2.29 Predicted: 3.54

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2-Chlorobenzoic acid Measured: 10.0 Predicted: 3.89

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2,6-Dichlorobenzoic acid

Measured: 1.82 Predicted: 3.59